

Universal Relation for the Inelastic Two-Body Loss Rate

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Abstract

Strongly-interacting systems consisting of particles that interact through a large scattering length satisfy universal relations that relate many of their central properties to the contact, which measures the number of pairs with small separations. We use the operator product expansion of quantum field theory to derive the universal relation for the inelastic 2-body loss rate. We verify the universal relation explicitly by direct calculations in the low-density limit at nonzero temperature. This universal relation can be tested experimentally using ultracold quantum gases of atoms in hyperfine states that have an inelastic spin-relaxation channel.

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I. INTRODUCTION

Atoms whose scattering length is large compared to the range of their interactions have universal properties that depend only on the large scattering length and are insensitive to details of their interactions at short distances [1]. These properties are universal in the sense that they apply to other types of nonrelativistic particles with short-range interactions, such as hadrons and nuclei, provided those particles have the same symmetries and mass ratios and large scattering lengths. The strong correlations associated with the large scattering length present challenges to understanding and calculating the properties of many-body systems of such particles. These challenges are particularly acute in the unitary limit in which the scattering length is infinite. This limit is characterized by scale invariance, so there are no well-defined quasiparticles upon which to base our understanding of the system.

Relations between various properties of a system that depend only on the large scattering length are called *universal relations*. Such relations provide powerful constraints on the behavior of the system that must be respected in spite of the strong correlations. Shina Tan derived a number of universal relations for the strongly-interacting two-component Fermi gas, which consists of two types of fermions that interact through a large scattering length [2–4]. These relations apply to any state of the system: few-body or many-body, homogeneous or trapped, normal or superfluid, balanced or polarized. For a few-body system, they apply as long as the energies relative to the appropriate threshold are small compared to the energy scale set by the range of the interactions. For a many-body system, they apply as long as the temperature and number density are small compared to the energy and density scales set by the range.

Tan’s universal relations all involve a property of the system C called the *contact* that measures the number of pairs of atoms of the two types with small separations. The contact is an extensive quantity that can be expressed as the integral over space of the contact density: $C = \int d^3r \mathcal{C}$. A convenient operational definition of the contact is provided by Tan’s *adiabatic relation*, which gives the rate of change of the total energy E of the system as the scattering length is varied [3]:

$$\frac{d}{da^{-1}} E = -\frac{\hbar^2}{8\pi\mu} C, \quad (1)$$

where μ is the reduced mass of the two types of atoms. If the system is at nonzero temperature, the derivative in Eq. (1) should be taken with the entropy held fixed. Using the adiabatic relation, any theoretical method that can be used to calculate the total energy of the system can also be used to calculate the contact. If the total energy can be measured in an experiment and if the scattering length can be controlled experimentally, for example by using a Feshbach resonance, the adiabatic relation can be used to measure the contact [5].

Tan derived his universal relations from the many-body Schrödinger equation by using generalized functions designed to implement the Bethe-Peierls boundary conditions associated with the large scattering length [2–4]. They were rederived by Braaten and Platter using the machinery of quantum field theory, specifically renormalization and the operator product expansion [6]. Tan’s universal relations make it clear that the contact plays a central role in the strongly-interacting Fermi gas. Subsequent work revealed that several of the most important experimental probes of ultracold atoms are related to the contact, including radio-frequency spectroscopy [7, 8] and photoassociation [9, 10]. A review of universal relations for fermions with a large scattering length was presented in Ref. [11].

One of the universal relations given in Ref. [11] is for the inelastic 2-body loss rate for fermions with a large scattering length. If atoms of types 1 and 2 have inelastic scattering channels with a large energy release, low-energy atoms will be lost from the system through inelastic collisions. Because of the inelastic scattering channels, the scattering length a must be complex with a negative imaginary part. The rate at which the number of either type of atom decreases is proportional to the contact:¹

$$\frac{d}{dt}N_\sigma = -\frac{\hbar}{4\pi\mu} \text{Im}(1/a) C. \quad (2)$$

The fact that the loss rate is proportional to C was first pointed out by Tan [12]. The prefactor of C in Eq. (2) was first written down by Braaten and Platter [6]. To the best of our knowledge, a derivation of Eq. (2) has not been presented previously. In this paper, we derive the universal relation for the 2-body loss rate using the operator product expansion of quantum field theory.

II. INELASTIC TWO-BODY LOSS

Inelastic two-atom scattering channels with a large energy release cause the loss of low-energy atoms from the system. The inelastic scattering channel may consist of lower hyperfine states of the atoms of types 1 and 2. The loss of low-energy atoms is actually due to their transformation into high-energy atoms. If the system is in a trapping potential, the high-energy atoms may have enough energy to escape from the trap. Even if they do not escape, their effects on the low-energy atoms can be neglected if their interactions with the low-energy atoms are weak enough. If the energy gap E_{gap} between the threshold for atoms 1 and 2 and the threshold for the final-state atoms is much larger than the low energies of interest, the inclusive effects of the inelastic collisions can be taken into account through anti-Hermitian terms in the Hamiltonian. These terms must be anti-Hermitian to account for the loss of probability from transitions of pairs of low-energy atoms to pairs of high-energy atoms, which are not taken into account explicitly.

An important consequence of the large energy gap E_{gap} is that there must be a small separation between the atoms of types 1 and 2 that disappear. By conservation of energy, the high-energy atoms created by the inelastic scattering of atoms of types 1 and 2 will emerge with large relative momentum that is approximately $(\mu E_{\text{gap}})^{1/2}$. By the uncertainty principle, the localized wave packet associated with each outgoing atom can be traced back to a region from which the atom emerged whose size is approximately $\hbar/(\mu E_{\text{gap}})^{1/2}$. But the two regions from which the two final-state atoms emerge must also be separated by a distance at most of order $\hbar/(\mu E_{\text{gap}})^{1/2}$, because the interactions that change the spin states of the atoms must also deliver a momentum kick of order $(\mu E_{\text{gap}})^{1/2}$. This large momentum can be transferred to the two final-state atoms only if they are close together. Even if the momentum is transferred through an intermediate atom in the original state 1 or 2, that atom must be far off its energy shell and therefore can propagate only over a short distance.

¹ The relation actually stated in Ref. [11] is that the rate of change of the number density n_σ is proportional to the contact density \mathcal{C} , which is not strictly correct. Integration over space is necessary to eliminate a term involving the divergence of the probability current.

The two atoms that disappear must therefore have a separation of order $(\mu E_{\text{gap}})^{1/2}$. Thus the non-Hermitian terms in the Hamiltonian must have short range.

III. DERIVATION OF THE UNIVERSAL RELATION

In this section, we derive the universal relation in Eq. (2) between the inelastic 2-atom loss rate and the contact. We use quantum field theory methods similar to those used in Ref. [6] to give concise derivations of other universal relations.

A. Quantum field theory

We begin by presenting the quantum field theory formulation of the problem of atoms with a large real scattering length a . We introduce quantum field operators $\psi_1(\mathbf{r})$ and $\psi_2(\mathbf{r})$ that annihilate atoms of type 1 and 2, respectively. If either atom is a boson, the fields satisfy the canonical commutation relations. If they are both fermions, they satisfy anticommutation relations. The masses of the atoms are m_1 and m_2 , and their reduced mass is $\mu = m_1 m_2 / (m_1 + m_2)$. The Hamiltonian operator for the system of atoms is the sum of a kinetic term, an interaction term, and possibly a term describing an external trapping potential: $\hat{H} = \hat{T} + \hat{U} + \hat{V}$. The kinetic and interaction terms can be expressed as

$$\hat{T} = \sum_{\sigma} \frac{1}{2m_{\sigma}} \int d^3r \nabla \psi_{\sigma}^{\dagger} \cdot \nabla \psi_{\sigma}(\mathbf{r}), \quad (3a)$$

$$\hat{U} = \frac{\hbar^2 g_0}{2\mu} \int d^3r \psi_1^{\dagger} \psi_2^{\dagger} \psi_2 \psi_1(\mathbf{r}), \quad (3b)$$

where g_0 is the bare coupling constant, which depends on the ultraviolet momentum cutoff Λ . The products of quantum field operators followed by the argument (\mathbf{r}) indicate that the operators are all evaluated at the same position \mathbf{r} . In the fermionic case, the ordering of the fields in the interaction term guarantees the positivity of the local operator. The ultraviolet cutoff can be implemented by limiting the Fourier transforms of the quantum field operators to wavenumbers satisfying $|\mathbf{k}| < \Lambda$. The scattering length for a pair of atoms of types 1 and 2 will have the value a if the bare coupling constant is chosen to be

$$g_0 = \frac{4\pi}{1/a - 2\Lambda/\pi}. \quad (4)$$

We now consider the problem of atoms that have inelastic scattering channels with a large energy gap. The large energy gap ensures that the anti-Hermitian terms in the Hamiltonian density must have a short range. We can therefore take them to be local operators involving the quantum fields ψ_1 and ψ_2 . Since the two atoms that disappear must have a very small separation, the appropriate operator is $\psi_1^{\dagger} \psi_2^{\dagger} \psi_2 \psi_1$, which annihilates a pair of particles at a point and then creates them again. This is precisely the operator in the interaction term of the Hamiltonian in Eq. (3b). To take account the loss of atoms, we can add such a term to the Hamiltonian with a coefficient that is pure imaginary and negative. Equivalently, we can simply take the bare coupling constant g_0 in Eq. (3b) to have a negative imaginary part. The inelastic scattering channel gives the scattering length a a negative imaginary part. The complex bare coupling constant g_0 can be obtained simply by inserting that complex scattering length a into Eq. (4).

B. Particle loss rate

We now consider the loss rate of the atoms. The time evolution of a state $|X(t)\rangle$ in the quantum field theory is given by

$$|X(t)\rangle = \exp(-i\hat{H}t/\hbar)|X(0)\rangle. \quad (5)$$

Because \hat{H} has a non-Hermitian part, the norm of the state $|X(t)\rangle$ decreases with time. The average number density of atoms of type σ in the state $|X(t)\rangle$ is given by the expectation value of the number density operator:

$$n_\sigma(\mathbf{r}, t) = \frac{\langle X(t)|\psi_\sigma^\dagger\psi_\sigma(\mathbf{r})|X(t)\rangle}{\langle X(t)|X(t)\rangle} \equiv \langle \psi_\sigma^\dagger\psi_\sigma(\mathbf{r}) \rangle. \quad (6)$$

Inserting the time evolution from Eq. (5) and differentiating with respect to time, we get

$$\frac{d}{dt}n_\sigma(\mathbf{r}, t) = \frac{i}{\hbar} \left(\langle \hat{H}^\dagger \psi_\sigma^\dagger\psi_\sigma(\mathbf{r}) - \psi_\sigma^\dagger\psi_\sigma(\mathbf{r}) \hat{H} \rangle - \langle \psi_\sigma^\dagger\psi_\sigma(\mathbf{r}) \rangle \langle \hat{H}^\dagger - \hat{H} \rangle \right). \quad (7)$$

The contribution from the kinetic term in the Hamiltonian can be expressed as the divergence of a current:

$$\langle [\hat{T}, \psi_\sigma^\dagger\psi_\sigma(\mathbf{r})] \rangle = i\hbar \nabla \cdot \langle \mathbf{J}_\sigma(\mathbf{r}) \rangle, \quad (8)$$

where \mathbf{J}_σ is the probability current operator for atoms of type σ :

$$\mathbf{J}_\sigma(\mathbf{r}) = -\frac{i\hbar}{2m_\sigma} (\psi_\sigma^\dagger \nabla \psi_\sigma(\mathbf{r}) - \nabla \psi_\sigma^\dagger \psi_\sigma(\mathbf{r})). \quad (9)$$

The flow term in Eq. (8) can be eliminated by integrating over all space and using the divergence theorem. The resulting expression for the rate of change of the total number of particles of type σ is

$$\frac{d}{dt}N_\sigma = \frac{i}{\hbar} \int d^3r \left(\langle \hat{U}^\dagger \psi_\sigma^\dagger\psi_\sigma(\mathbf{r}) - \psi_\sigma^\dagger\psi_\sigma(\mathbf{r}) \hat{U} \rangle - \langle \psi_\sigma^\dagger\psi_\sigma(\mathbf{r}) \rangle \langle \hat{U}^\dagger - \hat{U} \rangle \right), \quad (10)$$

where \hat{U} is the interaction energy operator in Eq. (3b). Using the (anti)commutation relations for the field operators, \hat{U} can be expressed in terms of the number density operators $\psi_1^\dagger\psi_1$ and $\psi_2^\dagger\psi_2$. It therefore commutes with $\psi_\sigma^\dagger\psi_\sigma(\mathbf{r})$. Thus only the non-Hermitian part of \hat{U} contributes to Eq. (10). The prefactor in $\hat{U}^\dagger - \hat{U}$ can be expressed as

$$\frac{\hbar^2(g_0^* - g_0)}{2\mu} = i \operatorname{Im}(1/a) \frac{\hbar^2|g_0|^2}{4\pi\mu}. \quad (11)$$

Thus the loss rate in Eq. (10) reduces to

$$\begin{aligned} \frac{d}{dt}N_\sigma = & -\frac{\hbar \operatorname{Im}(1/a)}{4\pi\mu} \int d^3r \int d^3r' \left(\langle |g_0|^2 \psi_1^\dagger \psi_2^\dagger \psi_2 \psi_1(\mathbf{r}') \psi_\sigma^\dagger \psi_\sigma(\mathbf{r}) \rangle \right. \\ & \left. - \langle |g_0|^2 \psi_1^\dagger \psi_2^\dagger \psi_2 \psi_1(\mathbf{r}') \rangle \langle \psi_\sigma^\dagger \psi_\sigma(\mathbf{r}) \rangle \right). \end{aligned} \quad (12)$$

We have combined the factor of $|g_0|^2$ with the operator $\psi_1^\dagger \psi_2^\dagger \psi_2 \psi_1$, because the dependence of matrix elements of this operator on the ultraviolet cutoff Λ is exactly cancelled by the Λ -dependence of $|g_0|^2$ [6]. The loss rate has been expressed in terms of a double integral over space of the connected part of the correlation function of two operators.

C. Operator product expansion

We proceed to use the operator product expansion to reduce the expression for the loss rate to single integrals over space of expectation values of local operators. If the separation $|\mathbf{r}' - \mathbf{r}|$ of the operators in the first term in the integrand in Eq. (12) is much larger than the correlation length of the system, the expectation value of the operator product factors into the product of the expectation values and it is therefore cancelled by the second term. Thus the integrand goes to zero as $|\mathbf{r}' - \mathbf{r}| \rightarrow \infty$. This motivates the expansion of the operator product in powers of $|\mathbf{r}' - \mathbf{r}|$:

$$|g_0|^2 \psi_1^\dagger \psi_2^\dagger \psi_2 \psi_1(\mathbf{r}') \psi_\sigma^\dagger \psi_\sigma(\mathbf{r}) = \delta^3(\mathbf{r}' - \mathbf{r}) |g_0|^2 \psi_1^\dagger \psi_2^\dagger \psi_2 \psi_1(\mathbf{r}) + \sum_n f_{\sigma n}(\mathbf{r}' - \mathbf{r}) \mathcal{O}_n(\mathbf{r}). \quad (13)$$

This operator equation is the *operator product expansion*. The sum is over local operators \mathcal{O}_n with increasingly higher scaling dimensions. The coefficients $f_{\sigma n}$ are functions of the separation vector $\mathbf{r}' - \mathbf{r}$ that depend on the scattering length a and the mass ratio m_1/m_2 . The coefficient of the leading operator is a Dirac delta function of $\mathbf{r}' - \mathbf{r}$. It can be derived simply by using the (anti)commutation relations for the field operators. The coefficients of higher dimension operators can be calculated using diagrammatic methods [6, 13]. Inserting the operator product expansion into Eq. (12), the loss rate reduces to

$$\frac{d}{dt} N_\sigma = -\frac{\hbar \text{Im}(1/a)}{4\pi\mu} \left(\int d^3r \langle |g_0|^2 \psi_1^\dagger \psi_2^\dagger \psi_2 \psi_1(\mathbf{r}) \rangle + \sum_n \int d^3r' f_{\sigma n}(\mathbf{r}') \int d^3r \langle \mathcal{O}_n(\mathbf{r}) \rangle \right). \quad (14)$$

The expectation value in the first integral on the right side can be identified as the contact density [6]:

$$\mathcal{C}(\mathbf{r}) = \langle |g_0|^2 \psi_1^\dagger \psi_2^\dagger \psi_2 \psi_1(\mathbf{r}) \rangle. \quad (15)$$

The additional terms involve integrals over space of expectation values of the local operators \mathcal{O}_n . Their coefficients $\int d^3r' f_{\sigma n}(\mathbf{r}')$ are functions of a and the mass ratio. Omitting the contributions in Eq. (14) from higher-dimension operators, we obtain the universal relation for the inelastic two-atom loss rate in Eq. (2).

The operator product expansion (OPE) in Eq. (13) is a systematic expansion in local operators with increasingly higher scaling dimension. The scaling dimension is a property of an operator that determines the behavior of its correlation functions at short distances. The correlation function $\langle \mathcal{O}(\mathbf{r}) \mathcal{O}'(\mathbf{r}') \rangle$ for a pair of local operators generally diverges as a power of the separation $|\mathbf{r} - \mathbf{r}'|$ as the separation vector approaches 0. The power is determined by the scaling dimensions of the operators. The quantum field operators ψ_σ and the number density operators $\psi_\sigma^\dagger \psi_\sigma$ have the naive scaling dimensions $\frac{3}{2}$ and 3 of a nonrelativistic free field theory. A gradient in an operator increases its scaling dimension by 1. For example, the kinetic energy operators $\nabla \psi_\sigma^\dagger \cdot \nabla \psi_\sigma$ have scaling dimension 5. A complete set of dimension-5 operators is listed in Ref. [15]. In a free field theory, the scaling dimension of a composite operator is the sum of the scaling dimensions of its factors. Thus the naive scaling dimension of $\psi_1^\dagger \psi_2^\dagger \psi_2 \psi_1$ is 6. However scaling dimensions can be strongly modified by interactions. In the case of a large scattering length, the scaling dimension of $\psi_1^\dagger \psi_2^\dagger \psi_2 \psi_1$ is reduced from 6 to 4 [14]. Three-body operators, which contain 3 quantum fields and their Hermitian conjugates, have non-integer scaling dimensions [14]. In the case

of fermions with equal masses ($m_1 = m_2$), the lowest-dimension 3-body operators that can appear in the OPE in Eq. (13) are $\mathcal{O}_\sigma^\dagger \cdot \mathcal{O}_\sigma$, where $\mathcal{O}_\sigma = 2\psi_2\psi_1\nabla\psi_\sigma - \psi_\sigma\nabla(\psi_2\psi_1)$ and σ is 1 or 2. They have scaling dimension 8.54 and the next higher operator has scaling dimension 9.33 [15]. In the case of unequal masses $m_1 < m_2$, the operator analogous to $\mathcal{O}_1^\dagger \cdot \mathcal{O}_1$ has a scaling dimension that decreases as m_2/m_1 increases. It reaches 5 at the critical value $m_2/m_1 = 13.6$ and remains at 5 for larger values of m_2/m_1 [15]. If atom 1 is a boson, the lowest-dimension 3-body operator that can appear in the OPE in Eq. (13) is $\psi_1^\dagger\psi_1^\dagger\psi_2^\dagger\psi_2\psi_1\psi_1$. The scaling dimensions of this operator is 5 for all values of the mass ratio m_2/m_1 .

We now consider which higher-dimension operators appear in the OPE for the loss rate in Eq. (14). The only operators that can contribute are those for which the integral over all space of the expectation value $\langle\mathcal{O}_n(\mathbf{r})\rangle$ is nonzero. Operators that are total derivatives have expectation values whose integrals are zero. If the system is homogeneous, only scalar operators have nonzero expectation values. If the system is static, operators that are total time derivatives have expectation values that are zero. Linear combinations of operators that vanish upon using the equations of motion for the quantum field operators also have zero expectation values. The additional operators that appear in the OPE in Eq. (14) are also limited to 3-body operators. This can be seen by using the (anti)commutation relations to normal order the quantum fields in the operator product in Eq. (13). The result is the sum of the first term on the right side and the normal-ordered form of the left side. But the normal-ordered operator has nonzero expectation value only in states that include 3 or more particles. Thus only 3-body and higher-body operators can appear in the additional terms in the loss rate in Eq. (14). The contact operator in Eq. (14) has scaling dimension 4. In the case of equal-mass fermions, the next term has an operator with scaling dimension 8.54. In the case of fermions with $m_2/m_1 > 13.6$ and in the case of bosons, the next term has an operator with scaling dimension 5.

We next determine how the coefficients $\int d^3r' f_{\sigma n}(\mathbf{r}')$ of the higher-dimension terms in the loss rate in Eq. (14) depend on a . The normalizations of the operators \mathcal{O}_n can be chosen so that their matrix elements have nontrivial unitary limits as $a \rightarrow \pm\infty$. A good example is the contact density operator $|g_0|^2\psi_1^\dagger\psi_2^\dagger\psi_2\psi_1$, for which the prefactor $|g_0|^2$ guarantees a well-behaved unitary limit. Given such operators, we can use dimensional analysis to determine how their coefficients depend on a . The first term inside the parentheses in Eq. (14) is the contact, which has dimensions 1/Length. If the operator \mathcal{O}_n has scaling dimension Δ_n , $\int d^3r \langle\mathcal{O}_n(\mathbf{r})\rangle$ has dimensions $(\text{Length})^{3-\Delta_n}$. By dimensional analysis, its coefficient $\int d^3r' f_{\sigma n}(\mathbf{r}')$ must have dimensions $(\text{Length})^{\Delta_n-4}$. Since a is the only dimensionful variable the coefficient depends on, $\int d^3r' f_{\sigma n}(\mathbf{r}')$ must be $|a|^{\Delta_n-4}$ multiplied by a numerical constant that depends only on the sign of a and on the mass ratio m_2/m_1 .

The truncation of the OPE for the loss rate in Eq. (14) to the leading term as in Eq. (2) is obviously a good approximation in the weak-coupling limit $a \rightarrow 0$. Let the largest important momentum scale for the system be $\hbar k_0$. Its contact is then of order k_0 . If \mathcal{O}_n has scaling dimension Δ_n , $\int d^3r \langle\mathcal{O}_n(\mathbf{r})\rangle$ will be at most of order $k_0^{\Delta_n-3}$. Multiplying by its coefficient, which is proportional to $|a|^{\Delta_n-4}$, we see that its contribution to the loss rate is suppressed by at least a factor of $(k_0|a|)^{\Delta_n-4}$. Thus, in the weak-coupling limit, the contributions from higher dimensions operators are parametrically suppressed by powers of $k_0|a|$. In the case of equal-mass fermions, the contribution to the loss rate from the first higher-dimension operator is suppressed by a factor of $(k_0|a|)^{4.54}$.

There are good reasons to believe that the truncation of the OPE for the loss rate in Eq. (14) remains a good approximation even near the unitary limit $a \rightarrow \pm\infty$. There is no

parametric suppression of higher dimension operators in this limit, so the validity of the truncation depends on the convergence properties of the OPE. The OPE was discovered independently by Kadanoff, Polyakov, and Wilson in 1969 [16–18]. Wilson proposed that the OPE was an asymptotic expansion in the small separation $|\mathbf{r} - \mathbf{r}'|$ of the operators [18]. Studies of the convergence of the OPE in relativistic quantum field theories suggest that it is actually a convergent expansion. Mack showed in 1977 that the OPE for a conformally-invariant field theory in 4 space-time dimensions converges for finite $|\mathbf{r} - \mathbf{r}'|$, at least when acting on the vacuum state [19]. More recently, Pappadopulo, Rychkov, Espin, and Rattazzi showed that the OPE for a conformal field theory in any space-time dimension not only has infinite radius of convergence in the separation $|\mathbf{r} - \mathbf{r}'|$, but the convergence at fixed $|\mathbf{r} - \mathbf{r}'|$ is actually exponential in the scaling dimension [20]. If the OPE is truncated by omitting terms with scaling dimension Δ_0 and higher, the error decreases like $\exp(-A\Delta_0)$, where A depends on the separation. Furthermore, Hollands and Koppen showed that the OPE for the simplest interacting scalar field theory in 4 space-time dimensions has similar convergence properties order by order in perturbation theory [21]. It has infinite radius of convergence in the separation $|\mathbf{r} - \mathbf{r}'|$, and the convergence at fixed $|\mathbf{r} - \mathbf{r}'|$ is exponential in the scaling dimension. If the OPE is truncated by omitting terms with scaling dimension Δ_0 and higher, the error decreases like $A^{\Delta_0}/(\Delta_0!)^{1/2}$, where A depends on the state and is proportional to the separation [21].

The convergence of the OPE in relativistic field theories does not guarantee its convergence in nonrelativistic field theories. However it is at least plausible that the OPE in a nonrelativistic field theory has infinite radius of convergence in the separation $|\mathbf{r} - \mathbf{r}'|$, and that the convergence at fixed $|\mathbf{r} - \mathbf{r}'|$ is exponential in the scaling dimension. This suggests that the OPE for the loss rate in Eq. (14) may have exponential convergence in the scaling dimension at any fixed scattering length, including the unitary limit $a = \pm\infty$. In the case of a balanced gas of equal-mass fermions at zero temperature near the unitary limit, the only important momentum scale is $\hbar k_F$, where $k_F = (3\pi^2 n)^{1/3}$. The contribution to the loss rate in Eq. (14) from an operator of scaling dimension Δ_n is not parametrically suppressed, but instead is enhanced by a factor of $(k_F |a|)^{\Delta_n - 4}$. However if the convergence is exponentially fast in the scaling dimension, the exponential factor $\exp(-A\Delta_n)$ overcomes the parametric enhancement. Thus the universal relation in Eq. (2) obtained by truncating the OPE after the leading term may be a good approximation even in the unitary limit.

IV. CONTACT IN THERMAL EQUILIBRIUM

In this section, we calculate the contact for a single pair of atoms in thermal equilibrium. We then use the result to obtain the contact density for a dilute gas of atoms or dimers. In this section, we take the scattering length a to be real and ignore the effects of inelastic scattering channels.

A. Single pair of atoms

We consider two atoms that are restricted to a volume V that is much larger than $|a|^3$ and are in thermal equilibrium at temperature T . The adiabatic relation in Eq. (1) can be used as an operational definition of the contact. It can be generalized to nonzero temperature by

taking the derivative with the entropy fixed. Equivalently, it can be expressed in the form

$$\frac{d}{da^{-1}} F = -\frac{\hbar^2}{8\pi\mu} C, \quad (16)$$

where F is the free energy and the derivative is taken with the temperature fixed. The free energy can be determined from the partition function:

$$Z = \exp(-\beta F), \quad (17)$$

where $\beta = 1/(k_B T)$. We will use the universal relation in Eq. (16) to calculate the contact for the single pair of atoms.

In the center-of-mass frame, the spectrum of the pair includes a continuum above the threshold from scattering states. Their energies can be parameterized as $E = \hbar^2 k^2 / (2\mu)$, where k is the wavenumber. The phase shift for an S-wave scattering state is

$$\delta(k) = -\arctan(ka). \quad (18)$$

If $a > 0$, the spectrum also has a discrete energy below the threshold: the dimer, whose energy is $E = -E_D$, where E_D is the binding energy:

$$E_D = \frac{\hbar^2}{2\mu a^2}. \quad (19)$$

Since the center-of-mass motion and the relative motion of the pair decouple, the partition function is the product of the associated partition functions Z_{cm} and Z_{rel} . The dependence on a enters only through Z_{rel} . In the limit $a \rightarrow 0^-$, there are no interactions and Z_{rel} reduces to the partition function for a free particle.

$$Z_{\text{free}} = V \int \frac{d^3 k}{(2\pi)^3} e^{-\beta \hbar^2 k^2 / (2\mu)} = V / \lambda_T^3, \quad (20)$$

where V is the spatial volume and λ_T is the thermal wavelength:

$$\lambda_T = \sqrt{\frac{2\pi\hbar^2}{\mu k_B T}}. \quad (21)$$

We express Z_{rel} as the sum of the free partition function in Eq. (20) and an interaction term that has all the dependence on a : $Z_{\text{rel}} = Z_{\text{free}} + Z_{\text{int}}$. The interaction term receives contributions from the continuum of S-wave scattering states and also, if $a > 0$, from the dimer. The spectrum of scattering states can be made discrete with energies E_n by making the spatial volume compact. A convenient method for discretizing the scattering states is to put the system in a spherical box with a large radius R . The interaction term can then be expressed as

$$Z_{\text{int}}(a) = \theta(a) e^{\beta E_D} + \sum_{n=1}^{\infty} e^{-\beta \hbar^2 k_n^2 / (2\mu)} - \sum_{n=1}^{\infty} e^{-\beta \hbar^2 k_n^2 / (2\mu)} \Big|_{a \rightarrow 0^-}. \quad (22)$$

The scattering wavefunctions $\sin[kr + \delta(k)]$ must satisfy the boundary condition

$$\sin[k_n R + \delta(k_n)] = 0. \quad (23)$$

Its nontrivial solutions satisfy

$$k_n R - \arctan(k_n a) = n\pi, \quad n = 1, 2, 3, \dots \quad (24)$$

In the limit $R \rightarrow \infty$, the discrete energies approach a continuum and the sum over integers approaches an integral:

$$\sum_{n=1}^{\infty} \rightarrow \frac{1}{\pi} \int_0^{\infty} dk \left(R - \frac{a}{1 + k^2 a^2} \right). \quad (25)$$

Inserting this into Eq. (22), we find that the dependence on R cancels and the interaction term reduces to

$$Z_{\text{int}} = \theta(a) e^{\beta \hbar^2 / (2\mu a^2)} - \frac{a}{\pi} \int_0^{\infty} dk \frac{1}{1 + k^2 a^2} e^{-\beta \hbar^2 k^2 / (2\mu)}. \quad (26)$$

The universal relation in Eq. (16) implies that the contact for the single pair of atoms is given by

$$C_{\text{pair}} = \frac{8\pi\mu}{\hbar^2 \beta} \frac{d}{da^{-1}} \log(Z_{\text{free}} + Z_{\text{int}}). \quad (27)$$

The derivative of Z_{int} is evaluated most easily if we first change the integration variable in Eq. (26) to the dimensionless variable $x = ak$. The resulting expression is

$$\frac{8\pi\mu}{\hbar^2 \beta} \frac{d}{da^{-1}} Z_{\text{int}} = \theta(a) \frac{8\pi}{a} e^{\beta \hbar^2 / (2\mu a^2)} + 8a^2 \int_0^{\infty} dk \frac{k^2}{1 + a^2 k^2} e^{-\beta \hbar^2 k^2 / (2\mu)}. \quad (28)$$

Our final result for the contact for a single pair of atoms is

$$C_{\text{pair}} = \frac{8\pi\mu}{\hbar^2 \beta} \frac{(d/da^{-1}) Z_{\text{int}}}{V/\lambda_T^3 + Z_{\text{int}}}, \quad (29)$$

where Z_{int} and its derivative are given in Eqs. (26) and (28). The integrals in these expressions can be evaluated analytically in terms of error functions.

The contact in Eq. (29) is for a pair of atoms in thermal equilibrium and also in chemical equilibrium with respect to transitions between a dimer and two unbound atoms. The contact for two unbound atoms that are not in chemical equilibrium with the dimer can be obtained by omitting the dimer contributions in the numerator and denominator of Eq. (29). In the large volume limit, we need only keep the first term in the denominator. The contact for the two unbound atoms reduces to

$$C_{AA} = \frac{8a^2 \lambda_T^3}{V} \int_0^{\infty} dk \frac{k^2}{1 + a^2 k^2} e^{-\beta \hbar^2 k^2 / (2\mu)}. \quad (30)$$

The contact for a dimer that is not in chemical equilibrium with unbound atoms can be obtained by keeping only the dimer terms in the numerator and denominator of Eq. (29). The result is extremely simple:

$$C_D = \frac{8\pi}{a}. \quad (31)$$

B. Dilute gas of atoms or dimers

We can use the expression in Eq. (30) for the contact for a single pair of unbound atoms to deduce the contact density for a homogeneous gas of atoms in the dilute limit. If the numbers of atoms in the volume V are N_1 and N_2 , the total number of pairs is $N_1 N_2$. Each pair gives the same contribution C_{AA} to the contact. We obtain the contact density by dividing by the volume: $\mathcal{C}_{AA} = N_1 N_2 C_{AA} / V$. Using the expression for C_{AA} in Eq. (30), we find that the contact density is proportional to the product of the number densities n_1 and n_2 :

$$\mathcal{C}_{AA} = 8a^2 \lambda_T^3 \left(\int_0^\infty dk \frac{k^2}{1 + a^2 k^2} e^{-\beta \hbar^2 k^2 / (2\mu)} \right) n_1 n_2. \quad (32)$$

We can use the expression in Eq. (31) for the contact C_D of a dimer to deduce the contact density for a homogeneous gas of dimers in the dilute limit. The total contact is C_D multiplied by the number N_D of dimers. We obtain the contact density by dividing by the volume. The result is proportional to the number density n_D of the dimers:

$$\mathcal{C}_D = \frac{8\pi}{a} n_D. \quad (33)$$

V. DIRECT CALCULATIONS OF INELASTIC LOSS RATES

In this section, we carry out direct calculations of inelastic loss rates for dilute homogeneous gases of atoms or dimers in thermal equilibrium. We take the scattering length a to be complex, with a negative imaginary part that takes into account inelastic scattering channels. For the direct calculations, it is more convenient to use the inverse scattering length $\gamma = 1/a$, which has a positive imaginary part.

A. Low-density gas of atoms

The elastic scattering amplitude for atoms with a large complex scattering length $a = 1/\gamma$ at wavenumber k is

$$f(k) = \frac{1}{-\gamma - ik}. \quad (34)$$

The differential cross section $|f(k)|^2$ is isotropic. The elastic cross section is obtained by multiplying it by the solid angle:

$$\sigma^{(\text{elastic})}(k) = \frac{4\pi}{|-\gamma - ik|^2}. \quad (35)$$

According to the optical theorem, the total cross section is the imaginary part of the forward scattering amplitude multiplied by $4\pi/k$:

$$\sigma^{(\text{total})}(k) = \frac{4\pi}{k} \text{Im} \left(\frac{1}{-\gamma - ik} \right). \quad (36)$$

The inelastic cross section is the difference between the total and elastic cross sections in Eqs. (36) and (35). The inelastic transition rate $g(k)$ per volume squared can be obtained by dividing the inelastic cross section by the flux factor $\mu/\hbar k$:

$$g(k) = \frac{4\pi\hbar}{\mu} \frac{\text{Im}(\gamma)}{|-\gamma - ik|^2}. \quad (37)$$

In the dilute limit, the inelastic loss rate can be written

$$\frac{d}{dt}n_1 = \frac{d}{dt}n_2 = -K_2 n_1 n_2, \quad (38)$$

where n_1 and n_2 denote the number densities of atoms 1 and 2, respectively. For an ensemble of particles 1 and 2, the inelastic loss rate coefficient K_2 can be calculated via a statistical average of the inelastic transition rate $g(k)$. Taking the ensemble to be atoms in thermal equilibrium at temperature T , the rate coefficient is

$$K_2 = \frac{\int d^3k e^{-\beta\hbar^2 k^2/(2\mu)} g(k)}{\int d^3k e^{-\beta\hbar^2 k^2/(2\mu)}} = \frac{\lambda_T^3}{2\pi^2} \int_0^\infty dk k^2 e^{-\beta\hbar^2 k^2/(2\mu)} g(k). \quad (39)$$

Inserting the inelastic transition rate $g(k)$ in Eq. (37), we obtain the loss rate coefficient K_2 :

$$K_2 = \frac{2\hbar\lambda_T^3}{\pi\mu} \text{Im}(\gamma) \int_0^\infty dk \frac{k^2}{|-\gamma - ik|^2} e^{-\beta\hbar^2 k^2/(2\mu)}. \quad (40)$$

According to the universal relation in Eq. (2), the right side of Eq. (38) must be proportional to the contact density:

$$K_2 n_1 n_2 = \frac{\hbar}{4\pi\mu} \text{Im}(1/a) \mathcal{C}_{AA}. \quad (41)$$

Comparing the expression for K_2 in Eq. (40) and \mathcal{C}_{AA} in Eq. (32), we see that they agree only to leading order in $\text{Im}(a)$. This is not surprising, because the contact density in Eq. (32) was calculated only for the case of real a . That calculation could presumably be extended to the case of complex a . The result must agree with Eq. (41) in the dilute limit. Thus the contact density in the dilute limit for atoms with a complex scattering length a must be

$$\mathcal{C}_{AA} = 8\lambda_T^3 \left(\int_0^\infty dk \frac{k^2 e^{-\beta\hbar^2 k^2/(2\mu)}}{|-1/a - ik|^2} \right) n_1 n_2. \quad (42)$$

B. Low-density gas of dimers

The inelastic loss rate for a dilute, noninteracting gas of dimers can be written as

$$\frac{d}{dt}n_D = -\Gamma_D n_D, \quad (43)$$

where Γ_D is the decay rate or inverse lifetime of the dimer. The decay rate can be expressed as an integral over momenta of the dimer wave function $\psi(k)$ in momentum space, its

complex conjugate $\psi^*(k')$, and the imaginary part of the two-particle-irreducible transition amplitude $U(k, k')$ for a pair of atoms:

$$\Gamma_D = \frac{2}{\hbar} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \psi(k) (-\text{Im } U(k, k')) \psi^*(k'). \quad (44)$$

In the field theory formulation of the problem with the interaction term in Eq. (3b), $U(k, k')$ is simply the bare coupling constant $g_0 \hbar^2/(2\mu)$. Since this is momentum independent, Γ_D simplifies to

$$\Gamma_D = \frac{\hbar}{\mu} (-\text{Im } g_0) \left| \int^{(\Lambda)} \frac{d^3k}{(2\pi)^3} \psi(k) \right|^2. \quad (45)$$

The normalized dimer wave function for complex scattering length $a = 1/\gamma$ is

$$\psi(k) = \frac{\sqrt{8\pi\text{Re}(\gamma)}}{\gamma^2 + k^2}. \quad (46)$$

If the integral in Eq. (45) was convergent, it would be the wave function at the origin in position space. However it is ultraviolet divergent, and it has therefore been regularized with a momentum cutoff Λ . The regularized integral is

$$\int_0^\Lambda \frac{k^2 dk}{2\pi^2} \psi(k) = \frac{\sqrt{8\pi\text{Re}(\gamma)}}{2\pi^2} (\Lambda - \gamma\pi/2). \quad (47)$$

This dependence on Λ is precisely what is required to cancel the Λ -dependence of the factor of $\text{Im } g_0$ in Eq. (45). The imaginary part of the coupling constant g_0 in Eq. (4) can be expressed as

$$\text{Im } g_0 = -\frac{\pi^3 \text{Im}(\gamma)}{|\Lambda - \gamma\pi/2|^2}. \quad (48)$$

Inserting Eqs. (48) and (47) into Eq. (45), we obtain a simple result for the decay rate:

$$\Gamma_D = \frac{2\hbar}{\mu} \text{Re}(\gamma) \text{Im}(\gamma) = \frac{2\hbar \text{Re}(a) \text{Im}(1/a)}{\mu|a|^2}. \quad (49)$$

This result for Γ_D can also be obtained from the expression for the dimer binding energy in Eq. (19) by analytically continuing the scattering length a to complex values. By expressing the complex energy $-\hbar^2/(2\mu a^2)$ in the form $-E_D - i\hbar\Gamma_D/2$, we can read off the width $\hbar\Gamma_D$ of the resonance. This prescription gives the same result for Γ_D as Eq. (49).

According to the universal relation in Eq. (2), the right side of Eq. (43) must be proportional to the contact density:

$$\Gamma_D n_D = \frac{\hbar}{4\pi\mu} \text{Im}(1/a) \mathcal{C}_D. \quad (50)$$

Comparing the expression for Γ_D in Eq. (49) and \mathcal{C}_D in Eq. (33), we see that they agree only to next-to-leading order in $\text{Im}(a)$. This is not surprising, because the contact density in Eq. (33) was calculated only for the case of real a . That calculation could presumably be extended to the case of complex a . The result must agree with Eq. (50) in the dilute

limit. Thus the contact density for a dilute gas of dimers in the case of a complex scattering length a must be

$$\mathcal{C}_D = \frac{8\pi \text{Re}(a)}{|a|^2} n_D. \quad (51)$$

Köhler, Tiesinga, and Julienne have derived a universal relation between the inelastic rate coefficient K_2 and the dimer lifetime $1/\Gamma_D$ [22]:²

$$K_2 = 2\pi a^3 \Gamma_D. \quad (52)$$

They considered the case in which $\text{Im}(a)$ is negligible compared to $\text{Re}(a)$. Using the expressions for K_2 in Eq. (40) and Γ_D in Eq. (49), we can see that the relation holds for K_2 in the zero-temperature limit and we can generalize it to a complex scattering length a :

$$K_2(T=0) = \frac{2\pi |a|^4}{\text{Re}(a)} \Gamma_D. \quad (53)$$

This differs from the relation for real a in Eq. (52) at next-to-next-to-leading order in $\text{Im}(a)$.

VI. TRAPPED GAS OF EQUAL-MASS FERMIONS

The universal relation for the inelastic two-body loss rate in Eq. (14) can be tested experimentally using atoms in hyperfine states that have an inelastic spin relaxation channel. Such an experiment has been carried out for identical bosons by Thompson, Hodby, and Wieman using an ultracold trapped thermal gas of ^{85}Rb atoms near a Feshbach resonance [23]. The results were interpreted theoretically by Köhler, Tiesinga, and Julienne in terms of the spontaneous dissociation of dimers [22]. The calculated lifetime of the dimers agreed well with the results extracted from the experiment except very close to the Feshbach resonance, where the predicted lifetime was too large. The extension of our universal relation for the atom loss rate to the case of identical bosons should allow a quantitative understanding of the loss rate much closer to the Feshbach resonance. Identical bosons introduce additional complications. One theoretical complication is that the operator product expansion analogous to Eq. (13) includes the 3-body contact operator, which has scaling dimension 5 [24]. The contribution from the 3-body contact may therefore not be strongly suppressed compared to the leading term from the 2-body contact. An experimental complication is that the contribution to the loss rate from 3-body recombination into the shallow dimer may also be important [23]. It is possible that part of the loss rate attributed to 3-body recombination in the experiment in Ref. [23] was actually due to the contact from unbound atoms.

An analogous experiment with equal-mass fermions would be particularly easy to interpret. The severe suppression of higher dimension operators implies that the simple universal relation in Eq. (2) should be very accurate. Additional contributions to the loss rate from 3-body recombination into the shallow dimer are also suppressed. The experiment could be carried out in the same way as the experiment with ^{85}Rb atoms in Ref. [23]. It would begin with a large number of atoms in thermal equilibrium at a scattering length on the

² This is the relation for fermions with two spin states. For identical bosons, the proportionality factor is $4\pi a^3$ [22].

negative side of a Feshbach resonance. The scattering length would then be ramped to a large positive value. The number of dimers that are produced could be controlled by varying the ramp rate. The scattering length would be held at the large positive value for a variable time, during which atoms and dimers could disappear. Finally, the scattering length would be ramped back to the negative side of the Feshbach resonance to dissociate the dimers, and the total number of remaining atoms would then be measured. By analyzing the dependence of the number of remaining atoms on the holding time, one could determine the contact for an unbound atom pair and/or the contact for a dimer. These contacts could be measured as functions of the scattering length and compared with the universal predictions.

We therefore consider a dilute gas of fermionic atoms and dimers that are trapped in a harmonic potential and in thermal equilibrium at a very low temperature T . We take the two types of atoms to be different spin states, so they have equal masses $m_1 = m_2 = m$, and we assume that they both feel the same trapping potential:

$$V(\mathbf{r}) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2). \quad (54)$$

The number densities n_1 and n_2 for the two spin states are Gaussians whose integrals over space are the total numbers of atoms N_1 and N_2 , respectively. The dimers feel the potential $2V(\mathbf{r})$. Their number density n_D is also a Gaussian whose integral over space is the total number of dimers N_D .

For simplicity, we assume that the imaginary part of the scattering length is extremely small compared to its real part. It therefore enters only in the prefactor of the contact in the universal relation in Eq. (14). The contact has contributions from unbound atoms and from dimers. The contribution from unbound atoms can be obtained by using the result for the contact density in Eq. (32) together with the local density approximation. It is obtained by integrating the contact density in Eq. (32) over all space. The result can be expressed as $N_1 N_2 C_{AA}$, where the contact for a single pair of atoms is

$$C_{AA} = 8a^2 \left(\frac{\hbar \bar{\omega}}{k_B T} \right)^3 \int_0^\infty dk \frac{k^2}{1 + a^2 k^2} e^{-\beta \hbar^2 k^2 / m} \quad (55)$$

and $\bar{\omega} = (\omega_x \omega_y \omega_z)^{1/3}$ is the geometric mean of the trapping frequencies. The contribution to the contact from dimers can be obtained by using the result for the contact density in Eq. (33) together with the local density approximation. Integrating the contact density over all space, we obtain the simple result $N_D C_D$, where $C_D = 8\pi a/m$ is the contact for a single dimer.

The number of dimers evolves independently from the number of unbound atoms. The time dependence for the number of dimers is

$$N_D(t) = N_D(0) \exp(-\Gamma_D t), \quad (56)$$

where $\Gamma_D = 4\hbar \text{Im}(1/a)/(ma)$. If the system is balanced, with equal numbers of atoms in the two spin states, the time dependence for the number of unbound atoms is also simple:

$$N_\sigma(t) = \left[\frac{1}{N_\sigma(0)} + \frac{\hbar \text{Im}(1/a)}{2\pi m} C_{AA} t \right]^{-1}, \quad (57)$$

where C_{AA} is the contact for a pair of unbound atoms in Eq. (55). If the initial number of dimers is sufficiently large, the loss rate will at first be dominated by the dimer contact.

However, as the dimers decay away, the loss rate will eventually be dominated by the contact from unbound atoms. The cross-over point at which the dominant loss mechanism changes from the dimer contact to the contact from unbound atoms is when the numbers of atoms and dimers satisfy $N_1 N_2 / N_D \approx C_D / C_{AA}$.

VII. SUMMARY

In summary, we have developed a rigorous theoretical framework for calculating the inelastic two-body loss rate for ultracold atoms with a large scattering length. We used the operator product expansion (OPE) to derive the universal relation for the inelastic two-body loss rate. The general result is given in Eq. (14) as an expansion in terms of integrals of expectation values of local operators with increasingly higher scaling dimensions. If we truncate the OPE to the leading term, we get the simple universal relation in Eq. (2) between the loss rate and the contact. In the weak-coupling limit in which the largest important momentum scale k_0 of the system satisfies $k_0 |a| \ll 1$, the OPE provides a systematically improvable approximation to the loss rate, because higher dimension terms are parametrically suppressed by powers of $k_0 |a|$. The truncation of the OPE to the leading term is particularly accurate in the case of fermions with equal masses, because the first correction is suppressed by a factor of $(k_0 |a|)^4$ ⁵⁴. If the OPE has the same convergence properties as in relativistic field theories, the general universal relation for the loss rate in Eq. (14) may remain useful near the unitary limit. The parametric enhancement of higher dimension terms by powers of $k_0 |a|$ could be overcome by numerical convergence factors that are exponential in the scaling dimension. This could justify the truncation of the OPE to the leading term, so the simple universal relation in Eq. (2) between the loss rate and the contact may be a good approximation even in the unitary limit.

We verified the universal relation by direct calculations for homogeneous gases of atoms and dimers in thermal equilibrium in the dilute limit. The contact density for a dilute gas of atoms is given in Eq. (32) for the case of a real scattering length and in Eq. (42) for the case of a complex scattering length. The corresponding results for a dilute gas of dimers are given in Eqs. (33) and (51).

We described how the universal relation in Eq. (2) could be tested using dilute ultracold gases of fermions with two spin states. The time dependence of the loss rate at a fixed scattering length could be used to measure both the contact for a single dimer and the contact for a pair of unbound atoms. The dependence of these contacts on the scattering length could then be compared with universal predictions. Agreement with the predictions would provide a beautiful illustration of how the universal relations constrain the interplay between few-body and many-body physics.

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